

Title: **Semiclassical Molecular Dynamics and its Implementation for Spectroscopic Calculations of High Dimensional and Condensed Phase Molecular Systems**

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Abstract:

I will present some novel semiclassical methods designed for spectroscopic calculations of high dimensional and/or condensed phase systems. Some of the methods are based on a “divide-and-conquer” approach, where the full dimensional spectra are obtained as a composition of several lower dimensional ones. Others exploit hierarchically the different levels of accuracy of different semiclassical propagators. All methods are within 10-20 wavenumbers Mean Absolute Error average respect to the exact or experiments when available, and are amenable to ab initio molecular dynamics simulations.

References

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